Project closing report (final report)

between 01-10-2013 and 30-09-2018

I. INTRODUCTION

In this project our research was to extended to novel types of materials which have recently become a central issue in condensed matter physics. With this aim we studied novel atomically thin nanostructures such as carbon based nanostructures (single and bilayer graphene), silicene, transition metal dichalcogenides, generalized two-dimensional Dirac electrons, topological insulators and its combination with conventional superconductors. We also investigated the unusual, multifractal nature of electronic states at or near quantum criticality. The dynamics of electrons and basic electronic properties of such systems was investigated by quantum mechanics. The project was a fundamental and theoretical research with great potential of applications.

During the funding period we have made used long term cooperations with C. J. Lambert, V. I. Fal'ko, Viktor Zólyomi from Lancaster (Lancaster University, UK), G. Burkard from University of Konstanz, B. Eckhardt, F. Gebhard and M. Kira from Marburg (Philipps University Marburg), with R. Moessner from Dresden (MPIPKS), with J. Cayssol from Berkeley (University of California) and with E. V. Castro and A. Cortijo from Madrid (ICMM), J. Ferrer from Universidad de Oviedo, Spain.

Fruitful works have been developed with several Hungarian research teams including the group of László Péter Biró and Levente Tapasztó, Katalin Kamarás, Balázs Újfalussy from Wigner Institute, and László Szunyogh, Szabolcs Csonka, András Halbritter, Ferenc Simon and Balázs Dóra from the Budapest University of Technology and Economics.

In this project the PI involved a few of his former PhD students, namely János Koltai, Andor Kormányos, András Pályi, László Oroszlány, Péter Rakyta, Gábor Szécshenyi, Gábor Csire, Máté Vigh and also with Norbert Barankai. Presently, two excellent PhD students: Gergő Kukucska and Zoltán Tajkov work in our group. Furthermore, in the funding period a few students started their BSc and MSc diploma thesis: Viktor Könye, Gábor Albrecht, Borbála Farkas, Eduard Jurca, Noel Plaszkó, and in the last year a fresh year BSc student Róbert Németh.

Below we review the scientific works done during the funding period taking into account the subjects we proposed originally in our project. The references here are just a selection of that submitted in the NKFI Office and it only serves to guide the Referee(s).

II. ELECTRONIC STRUCTURE AND TRANSPORT PROPERTIES OF ATOMICALLY THIN CARBON BASED NANOSTRUCTURES AND TRANSITION METAL DICHALCOGENIDES

During the supported period we studied the surface states of topological insulators using the multiple scattering theory. During our work we examined the electrostatic properties of the surface states as a function of the concentration of the charged impurities localized close to the surface of the crystal.

In addition, we also studied the transport properties of graphene based nanostructures. Our studies were conducted in cooperation with local experimental groups and were focused on experimentally relevant structures. We have shown, that bound states localized inside the bulk of graphene based junctions [1, 2] can induce scattering processes between the Hall states propagating over the edges [1].

We also studied the transport properties of transitional metal dichalcogenide materials. In our work [3] we have developed a low energy two-band model that can describe both the magnetic valley splitting and the trigonal warping of the energy bands close to the K points. Using this model we examined the Shubnikov-de-Haas oscillations as a function of the magnetic splitting of the valleys.

Moreover, we developed a numerical approach to calculate the equilibrium Josephson effect that can be applied to describe the Josephson effect in experimentally relevant systems. Using our approach we examined the magnetic oscillations of the critical current in long Josephson junctions [4]. In addition, we also studied Fabry-Pérot oscillations in graphene based Josephson junctions [5]. Our theoretical results were in good agreement with the experimental results obtained by our experimental colleagues from Delft, the Netherlands.

We present a theoretical study of the spin-valley blockade transport effect in a double quantum dot defined in a straight [6] and bent [7] carbon nanotube. The electrical current flowing through quantum dots especially sensitive to small variations of the external magnetic field, so a carbon nanotube-based device can be used to measure magnetic fields with high sensitivity $\left(1\mu\mathrm{T}/\sqrt{Hz}\right)$ [8].

During the funding period we made several advances in the study of nanoelectronics [9–14] and nanomagnetism [15–19], we also explored the role of novel topological phases [10, 12, 20, 21] in recent experiments.

Focusing on nanoelectronics, new theoretical tools were developed for investigating electronic transport [9] in model systems [12], graphene based devices with strong spin orbit coupling [11], molecular break junctions [14] and topological heterostructures [10]. Our results underpinned the experimental work in András Halbritter and Szabolcs Csonka's research group at Budapest University of Technology and Economics (BUTE).

In a strong collaboration with the research group of Laszló Szunyogh at the BUTE the study of magnetic properties of nanodevices was carried out [15–19]. We implemented tools to investigate strongly correlated systems [18] and a novel approach to extract magnetic model parameters from *ab initio* calculations employing a non orthogonal basis set [19]. We applied the developed tools to the study of magnetic multilayers [15–17] and graphene based exotic magnetic systems [19].

Topological phases represent one of the most intriguing discovery of recent years. The surface states (in other words edge states) of the topological insulators corresponding to the electrons moving along the surface of the material are symmetry-protected by particle number conservation and time reversal symmetry. Recently, J. Asbóth, L. Oroszlány (member of the present project), and A. Pályi have published an introductory book for students and researchers on topological insulators to provide a basic understanding of edge states, bulk topological invariants, and of the bulk–boundary correspondence with as simple mathematical tools as possible [20].

The topological phase diagram and transport properties of graphene based hybrid systems was investigated in the publication [10]. The electronic properties of topological semimetals in two dimensions were studied by numerical and theoretical means in [12]. The magnetic response of the recently discovered nodal loop semimetals was investigated in [21], our study explains hitherto ununderstood experimental findings in these novel topological materials.

In publications [13] and [21] materials and physical properties were explored where the exotic structure of the spin-orbit coupling leads to novel topological phases. Manuscript [13] details the results of a fruitful collaboration with experimentalists where we report the first isolation of a single layer of BiTeI monolayer. The performed ab-initio calculations and experimental findings unequivocally confirmed the presence of this new two-dimensional material. In [21] signatures of possible topological phase transitions were examined in magneto oscillation spectra of nodal loop semimetals. It was found that depending on the direction of the magnetic field two regimes can be separated. In one regime only oscillations with trivial Berry phases manifest, while in the other a mixture of trivial and topological oscillations can coexist. This study explains hitherto understood experimental findings in these novel materials. In publications [15, 16] the properties of magnetic layers and interfaces were studied. In [15] the demagnetisation process in Fe/Ir/Fe sandwiches is shown to be much slower at the interface as compared with the bulk, a key insight to interpret ultrafast laser-induced demagnetization processes in layered or interface materials. In [16] Fe/MgO-based magnetic tunnel junctions were investigated. These systems are promising candidates for spintronic devices due to their high thermal stability and high tunneling magnetoresistance. Our results demonstrate the intrinsic physical complexity of the pure Fe/MgO interface and the role of elevated temperatures providing insight when interpreting experimental data of nanoscale magnetic tunnel junctions. Finally, in [19] a new method for obtaining magnetic model parameters was discussed. We have shown that Lichtenstein's approach can be generalized to first principles calculations employing nonorthogonal basis sets. We demonstrated that our approach gives the same spin model parameters as those obtained by the KKR approach for elementary metals.

III. ELECTRIC CONDUCTIVITY OF THE GENERALIZED TWO-DIMENSIONAL DIRAC ELECTRONS AND THE TIME EVALUATION OF THE TOPOLOGICAL STATES

A quadratic band crossing in two dimensions is known to have a generic instability towards a quantum anomalous Hall (QAH) ground state for infinitesimal repulsive interactions. We introduced a generalization of a quadratic band crossing which is protected only by rotational symmetry, and found that the interaction induced nematic phase can compete successfully with the QAH insulator, and to become the dominant instability in certain parts of the phase diagram already at weak coupling [22].

We have further generalized this model to a quadratic+flat band touching [23]. The Landau level structure in a quantizing magnetic field and the longitudinal and transversal magneto-optical conductivities were calculated. The Hall conductivity from each valley is rational (not quantized at all), in agreement with Berry phase considerations, though their sum is always integer quantized.

We also studied the equilibrium and quench properties of two dimensional fermions with quadratic band touching at the Fermi level, in the presence of infinitely long range interactions [24]. Unlike when only short range interactions are present, both nematic and quantum anomalous Hall (QAH) states state appear at weak interactions, separated by a narrow coexistence region. After an interaction quench, the QAH order exhibits three distinct regions: persistent or damped oscillations and exponential decay to zero. In contrast, the nematic order always reaches a non-zero stationary value through power law damped oscillations, due to the interplay of the symmetry of the interaction and the specific topology of the quadratic band touching.

Parallel to these developments, we have focused on the fate of topological states of matter after a quantum quench, with special emphasis on dynamical quantum phase transitions (DPT). These are signalled by the non-analytical time evolution of the dynamical free energy, which is calculated from the Loschmidt overlap between the initial and time evolved states. By studying a minimal model, the XY chain in transverse magnetic field, we presented examples where DPT occurs without crossing any equilibrium critical lines by the quench, and a nontrivial example with no DPT but crossing a critical line by the quench. Albeit the non-analyticities of the dynamical free energy on the real time axis do not indicate the presence or absence of an equilibrium phase transition, the structure of Fisher-lines for complex times reveal a qualitative difference [25]. We have shown that the time evolution of the dynamical free energy is crucially affected by the ground state topology of both the initial and final Hamiltonians, implying DPTs when the topology is changed under the quench. Similarly to edge states in topological insulators, DPTs can be classified as being topologically protected or not.

In 1D systems the number of topologically protected non-equilibrium time scales are determined by the difference between the initial and final winding numbers, while in 2D no such relation exists for the Chern numbers [26]. In 1D, Luttinger liquids (LLs) arise by coupling left- and right-moving particles through interactions in one dimension. This most natural partitioning of LLs was investigated by the momentum-space entanglement after a quantum quench [27, 28]. The largest entanglement eigenvalue is identical to the Loschmidt echo, i.e. the overlap of the disentangled and final wavefunctions of the system. The entanglement gap is universal both in equilibrium and after a quantum quench. The momentum–space entanglement entropy is always extensive and saturates fast to a time independent value after the quench, in sharp contrast to a spatial bipartitioning. Information scrambling and the butterfly effect in chaotic quantum systems can be diagnosed by out-of-time-ordered (OTO) commutators through an exponential growth and large late time value. We have studied this quantity for Luttinger liquids [29] and for the transverse field Ising chain [30], and demonstrated that the OTO commutator can be used to detect DTPs, and non-Fermi liquids can behave in many respect as chaotic systems.

IV. FIRST PRINCIPLES STUDY OF ATOMICALLY THIN STRUCTURES

We have performed an empirical reparametrization of the HSE06 exact exchange density functional by fitting the amount of exact exchange and screening in the functional in order to achieve the closest match possible to the many-body corrected GW calculations. For fitting the parameters two benchmark materials were considered diamond and β-silicon carbide. We have demonstrated that this method is sound and accurate, as our modified HSE functional performs very well in three-dimensional materials such as bulk silicon, germanium, gallium arsenide, cadmium telluride or low-dimensional systems like molybdenum disulphide, hexagonal boron nitride and single-walled carbon nanotubes. Since the modified HSE functional is a significantly cheaper method than the GW approximation, being both a better-scaling and, more importantly, a faster-converging method, our functional can be used to perform calculations on the kind of large systems that cannot be feasibly treated in GW while approaching the accuracy of GW at the same time [31] (unfortunately in this paper the NKFI-ID is missing in the acknowledgment).

In fact, in some cases even performing computation with the modified HSE functional is too expensive, therefore we constructed tight binding Hamiltonians fitted to HSE calculations on 2D layered, hexagonal materials. The Hamiltonian was built by using the Slater-Koster method, taking up to third-nearest neighbour hopping interaction into account. Considering the symmetries of the systems, we reduced the number of parameters significantly. During the fitting procedure we acquired several parameter sets using the least squares approach, which reproduced the first principles band structures fairly well. As an application we consider electronic and optical properties of silicene or germanene (see Refs. [32, 33] in Chapter V).

V. OPTICAL PROPERTIES OF NOVEL TWO DIMENSIONAL CRYSTALS WITH/WITHOUT DISORDER AND/OR DEFECTS, STUDIES OF THE DISORDER AND DEFECTS IN GENERAL

In [34] we develop a general method to calculate the optical rotation of the polarization of light incident on multilayer systems consisting of atomically thin conductors and dielectric multilayers. As a demonstration we calculate the Kerr (Faraday) angle for bilayer graphene in the quantum anomalous Hall state placed on the top of dielectric multilayers.

By means of this tight-binding Hamiltonian we calculated electronic and optical properties of silicene or germanene We present a third-nearest neighbour tight-binding model parametrized from first principles density functional theory and use it to describe Raman processes involving scattering of quasiparticles by phonons or point defect in silicene or germanene [33]. Furthermore, Gregő Kukucska has a detailed account on this issue in his PhD thesis submitted just recently [32].

We investigate the fate of the flat band in the presence of disorder by focusing on the density of states (DOS) and dc conductivity for lattices, such as the dice or the Lieb lattice, possessing Dirac cones with a flat band crossing the Dirac point, and for which the effective model is a pseudospin-1 Dirac-Weyl Hamiltonian [12].

In [35] we theoretically study a single-electron spin-valley qubit in an electrostatically defined quantum dot in a transition metal dichalcogenide monolayer, focusing on the example of MoS2. Tilted magnetic field together with a short-range impurity can give rise to a coupling between the qubit basis states. We reveal highly unconventional features of this coupling mechanism, arising from symmetry-forbidden intervalley scattering, in the case when the impurity is located at a S site.

Performing frequent measurements on a quantum system, in order to determine whether it is in a particular subspace, forces the system to remain in that subspace. This fact is related to the quantum information processing tasks, e.g., active decoherence avoidance and error correction. In [36] we give a generalization of previous results concerning propagators with possibly time-dependent generators acting on Banach spaces.

The phase diagram of the metal-insulator transition in a three-dimensional quantum percolation problem is investigated numerically based on the multifractal analysis of the eigenstates. The large-scale numerical simulation has been performed on systems with linear sizes up to $L = 140$. The multifractal dimensions, exponents D_q and α_q, have been determined in the range of $0 \leq q \leq 1$. Our results confirm that this problem belongs to the same universality class as the three-dimensional Anderson model; the critical exponent of the localization length was found to be $\nu = 1.622 \pm 0.035$. However, the multifractal function $f(\alpha)$ and the exponents D_q and α_q produced anomalous variations along the phase boundary, $p_c^Q(E)$ [37].

The application of the technique developed in the case of quantum percolation enabled us to perform further simulations of the disorder-induced metal-insulator transition in a three-dimensional simple cubic lattice and compared for the presence and absence of time-reversal and spin-rotational symmetry, i.e., in the three conventional symmetry classes. Large-scale numerical simulations have been performed on systems with linear sizes up to $L = 100$ in order to obtain eigenstates at the band center, $E = 0$. The multifractal dimensions, exponents D_q and α_q, have been determined in the range of $-1 \leq q \leq 2$. The finite-size scaling of the generalized multifractal exponents provide the critical exponents for the different symmetry classes in accordance with values known from the literature based on high-precision transfer matrix techniques. The multifractal exponents of the different symmetry classes provide further characterization of the Anderson transition, which was missing from the literature so far. As a result the precision achieved competes with the ones obtained using conventional transfer matrix technology and recently our work has become a benchmark for subsequent investigations of similar systems [38].

Recently, based on heuristic arguments, it was conjectured that an intimate relation exists between any multifractal dimensions, Dq and $D_{q'}$, of the eigenstates of critical random matrix ensembles: $D_{q'} \approx qD_q[q' + (q - q')D_q]^{-1}$, $1 \leq q \leq 2$. Here, we verify this relation by extensive numerical calculations on critical random matrix ensembles and extend its applicability to $q < 1/2$, but also to deterministic models producing multifractal eigenstates and to generic multifractal structures. We also demonstrate, for the scattering version of the power-law banded random matrix model at criticality, that the scaling exponents q of the inverse moments of Wigner delay times, $\langle \tau_{\mathrm{W}}^{-q} \rangle \propto N^{-\sigma_q}$ where N is the linear size of the system, are related to the level compressibility χ as $\sigma_q \approx q(1-\chi)[1+q\chi]^{-1}$ for a limited range of q, thus providing a way to probe level correlations by means of scattering experiments [39].

An interesting outreach of the technique developed by us is the investigation of the Anderson transition found in the spectrum of the Dirac operator of quantum chromodynamics at high temperature, studying the properties of the critical quark eigenfunctions. Applying multifractal finite-size scaling we determine the critical point and the critical exponent of the transition, finding agreement with previous results, and with available results for the unitary Anderson model. We estimate several multifractal exponents, finding also in this case agreement with a recent determination for the unitary Anderson model. Our results confirm the presence of a true Anderson localization-delocalization transition in the spectrum of the quark Dirac operator at high temperature, and further support that it belongs to the 3D unitary Anderson model class [40].

We perform a detailed numerical study of the conductance G through one-dimensional (1D) tight-binding wires with on-site disorder. The random configurations of the on-site energies ϵ of the tight-binding Hamiltonian are characterized by long-tailed distributions: For large ϵ, $P(\epsilon) \sim 1/\epsilon^{1+\alpha}$ with $\alpha \in (0, 2)$. Our model serves as a generalization of the 1D Lloyd model, which corresponds to $\alpha = 1$. First, we verify that the ensemble average $< -\ln G >$ is proportional to the length of the wire L for all values of α, providing the localization length ξ from $< -\ln G >= 2L/\xi$. Then, we show that the probability distribution function $P(G)$ is fully determined by the exponent α and $< -\ln G >$. In contrast to 1D wires with standard white-noise disorder, our wire model exhibits bimodal distributions of the conductance with peaks at $G = 0$ and 1. In addition, we show that $P(\ln G)$ is proportional to G^β for $G \to 0$, with $\beta \leq \alpha/2$, in agreement with previous studies [41].

VI. SUMMARY

Recently, the PI and several researchers of the present project have been established the Eötvös Quantum Transport Group in the Institute of Physics of the Eötvös Loránd University. In our theoretical works we have used the free Eötvös Quantum Transport Utilities (EQuUs) software package developed by the Eötvös Quantum Transport Group. Our software implementation package includes all the numerical algorithms that are the most effective versions in the literature. Thus, our enhanced numerical capacity enables us to address such questions that can be relevant for applications and to experimental researchers. In this way, working with experimental groups the task for our research team is to provide a physical interpretation and deeper understanding of the experimental results.

Based on the fruitful collaboration established recently with experimental groups at Kavli Institute of Nanoscience and QuTech, Delft University of Technology, The Netherlands [5], and at Budapest University of Technology and Economics in Hungary our theoretical works may initiate new directions in applications and experimental research [1, 13, 14]. Ongoing collaborations exist with experimental groups from Wigner Research Centre for Physics and The Institute of Technical Physics and Materials Science (MFA). Moreover, last year PI and many of the member of our Eötvös Quantum Transport Group joined to the National Quantum Technology Program, The HunQuTech consortium (see here) implemented with the collaboration of academic, University and business research centres.

We hope that our theoretical research indicated above can be a firm basis in the future for a high standard research in Hungary at the international level in a rather new and unique research field of the atomically thin materials.

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